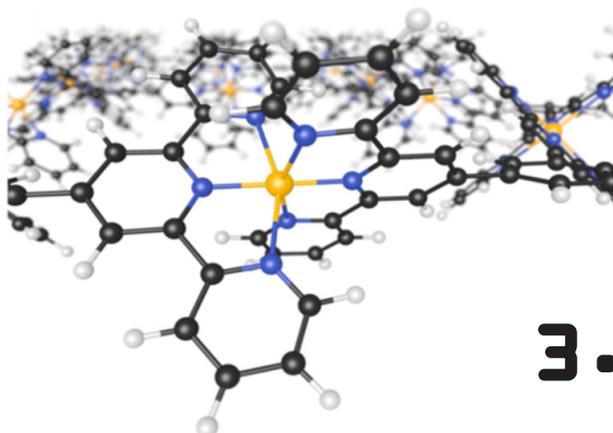
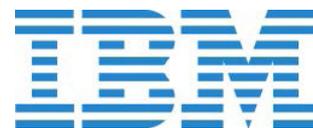




University of  
Zurich<sup>UZH</sup>

**ETH**

Eidgenössische Technische Hochschule Zürich  
Swiss Federal Institute of Technology Zurich



## 3.C4-Workshop

Friday, 13 October 2017

Universität Zürich, Campus Irchel

Lecture Hall 15 G 19

### Program

**13:00 Lubomir Rulisek, CAS Prag**

*Striving for Quantitative Accuracy in Computations of Thermodynamic, Kinetic, and Spectroscopic Properties of Bioinorganic Systems*

**13:40 Marc van der Kamp, University of Bristol**

*Multi-scale simulation of enzymes: Details of mechanisms and efficient in silico screening*

**14:20 Marwin Segler, Westfälische Wilhelms-Universität, Münster**

*Retrosynthesis and Reaction Prediction with Modern Artificial Intelligence*

**15:00 Coffee Break**

**15:30 David Tew, Max-Planck-Institut für Festkörperforschung, Stuttgart**

*Accurate wavefunctions for large molecular systems*

**16:10 Thomas Kühne, University of Paderborn**

*Metal-Insulator Transition of solid Hydrogen by a Fermionic Shadow Wave Function*

**17:00 Apéro**